

## WEST Search History

DATE: Sunday, March 21, 2004

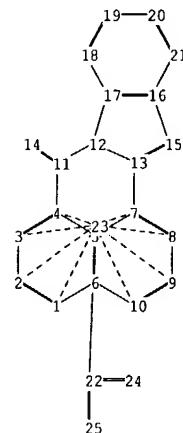
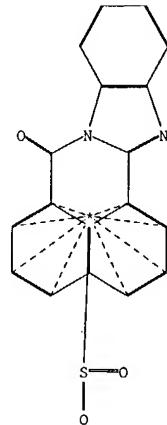
Hide? Set Name Query

Hit Count

*DB=USPT,EPAB,JPAB,DWPI,TDBD; PLUR=NO; OP=ADJ*

|                          |    |   |   |
|--------------------------|----|---|---|
| <input type="checkbox"/> | L3 | us-2949467-\$ did. or us-4024144-\$ did. or us-5470921-\$ did.    | 6 |
| <input type="checkbox"/> | L2 | us-6583284-\$ did.  | 2 |
| <input type="checkbox"/> | L1 | jp-51111237-\$ did. or jp-52072726-\$ did. or jp-58057463-\$ did. | 6 |

END OF SEARCH HISTORY



**chain nodes :**

14 22 24 25

**ring nodes :**

1 2 3 4 5 6 7 8 9 10 11 12 13 15 16 17 18 19 20 21

**chain bonds :**

11-14 22-24 22-25

**ring bonds :**

1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-13 8-9 9-10 11-12 12-13 12-17  
13-15 15-16 16-17 16-21 17-18 18-19 19-20 20-21

**exact/norm bonds :**

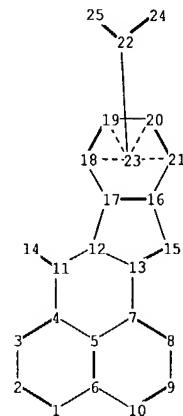
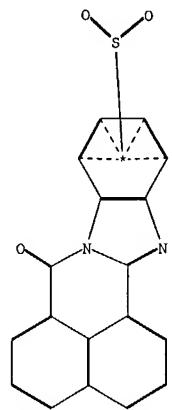
4-11 7-13 11-12 11-14 12-13 12-17 13-15 15-16 22-24 22-25

**normalized bonds :**

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19  
19-20 20-21

**Match level :**

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:CLASS 23:CLASS 24:CLASS 25:CLASS



chain nodes :

14 22 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 15 16 17 18 19 20 21

chain bonds :

11-14 22-24 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-13 8-9 9-10 11-12 12-13 12-17  
13-15 15-16 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

4-11 7-13 11-12 11-14 12-13 12-17 13-15 15-16 22-24 22-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19  
19-20 20-21

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:CLASS 23:CLASS 24:CLASS 25:CLASS

=> d his

(FILE 'HOME' ENTERED AT 19:32:35 ON 21 MAR 2004)

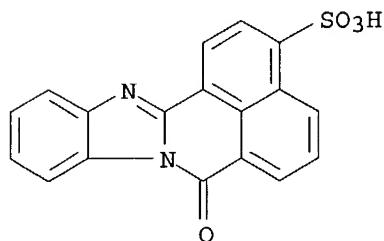
FILE 'REGISTRY' ENTERED AT 19:32:42 ON 21 MAR 2004

L1                   STRUCTURE UPLOADED  
L2                   STRUCTURE UPLOADED  
L3                   19 S L1 OR L2  
L4                   STRUCTURE UPLOADED  
L5                   STRUCTURE UPLOADED  
L6                   4 S L4 OR L5  
L7                   112 S L4 OR L5 FUL

RN 41537-57-9 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3-sulfonic acid, 7-oxo-, sodium salt (9CI) (CA INDEX NAME)  
 MF C18 H10 N2 O4 S . Na  
 LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier | RID Occurrence |
|--------------------|--------------------|-------------------|---------------------|-----------------|----------------|
| EA                 | ES                 | SZ                | RF                  | RID             | Count          |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3        | 1              |
| C6-C6              | C6-C6              |                   |                     |                 |                |



● Na

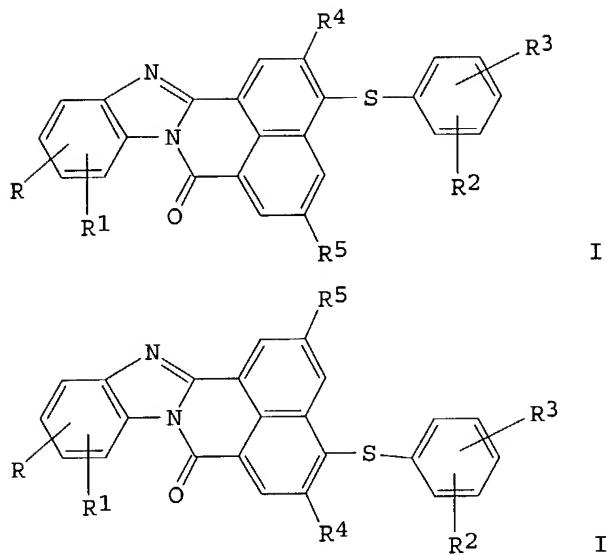
2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:191337 CA  
 TI 1,8-Naphthylenebenzimidazole derivatives  
 IN Shiroasaki, Tsutomu  
 PA Nippon Kayaku Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC C09B057-00  
 CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)  
 Section cross-reference(s): 28

FAN.CNT 1

|      | PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|------|---------------|------|----------|-----------------|----------|
| PI   | JP 51111237   | A2   | 19761001 | JP 1975-36069   | 19750327 |
| PRAI | JP 1975-36069 |      | 19750327 |                 |          |
| GI   |               |      |          |                 |          |



AB I-II mixts. ( $R = H, Me, OMe, Bu, NO_2, Cl, CO_2H; R1 = H, Me; R2 = H, NH_2, Bu, Me, OMe; R3 = H, Cl, Me, CO_2H; R4 = H, Cl, Br, OH, OMe, OPr; R5 = H, Cl, Br, OH, OMe, OPr, NO_2, SO_2NMe_2, SO_2NET_2$ ) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared. For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at  $98^\circ$  for 12 h and then autoclaved with 2-aminobenzethiol [137-07-5] in the presence of  $K_2CO_3$  and  $Na_2SO_3 \cdot 7H_2O$  at  $150^\circ$  for 10 h and at  $170^\circ$  for 12 h to give I-II mixture (all  $R$ 's =  $H$  except  $R2 = 2-NH_2$ ); about 34 I-II mixts. were prepared.

ST phenylthionaphthoylenebenzimidazole deriv manuf; naphthoylenebenzimidazole phenylthio deriv

IT Dyes  
(intermediates, (phenylthio)naphthoylenebenzimidazole derivs.)

IT 41537-57-9P 62602-99-7P  
RL: PREP (Preparation)  
(manufacture and reaction with aminobenzethiol)

IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P  
RL: PREP (Preparation)  
(manufacture and reaction with aminomethylbenzethiol)

IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P  
62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P  
62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P  
62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P  
62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P  
62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P  
62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P  
62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P  
62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P  
62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P  
62599-24-0P 62599-25-1P 62599-26-2P 62599-27-3P 62599-28-4P  
62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P  
62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P  
62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of)

IT 62635-64-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with benzenediamine)

IT 95-54-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sulfonaphthalic anhydride sodium salt)  
IT 106-45-6 137-07-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole)  
IT 2396-68-1 23451-96-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole derivs.)

REFERENCE 2

AN 78:124591 CA  
TI Hydrazinoperinones  
IN Okada, Hiroshi; Kaneko, Masaharu; Kato, Yoshiaki  
PA Mitsubishi Chemical Industries Co., Ltd.  
SO Jpn. Kokai Tokyo Koho, 5 pp.  
CODEN: JKXXAF  
DT Patent  
LA Japanese  
NCL 16E6  
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))  
FAN.CNT 1

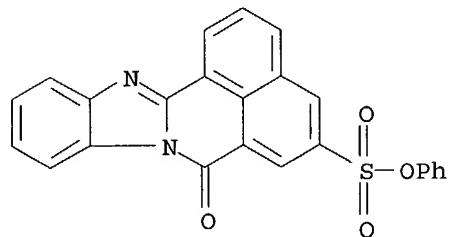
| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|-------------|------|----------|-----------------|----------|
| JP 48013385 | B4   | 19730220 | JP 1971-42394   | 19710614 |
| JP 50036447 |      | 19750000 | JP              |          |

GI For diagram(s), see printed CA Issue.  
AB The title compds. (I where X = NHNH<sub>2</sub>), dye and pigment intermediates, were prepared E.g., 7.5 g I (X = SO<sub>3</sub>Na, Y = H) in H<sub>2</sub>O was refluxed 6 hr with 4 g N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O to give 5 g I (X = NHNH<sub>2</sub>, Y = H). Similarly prepared were the following I (X = NHNH<sub>2</sub>) (Y given): x-Cl; x-NO<sub>2</sub>; x-OMe; x-Me. Also prepared were II and III.  
ST hydrazinoperinone dye intermediate; perinone hydrazino dye intermediate  
IT Dyes  
Pigments  
(intermediates for, hydrazinoperinones derivs. as)  
IT 41537-58-0P 41537-59-1P 41537-60-4P 41576-18-5P 41576-19-6P  
41576-20-9P 41576-21-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 41537-57-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with hydrazine)

RN 58373-92-5 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 10(or  
   11)-ethoxy-7-oxo-, phenyl ester (9CI) (CA INDEX NAME)  
 MF C26 H18 N2 O5 S  
 CI IDS  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier | RID Occurrence |
|--------------------|--------------------|-------------------|---------------------|-----------------|----------------|
| EA                 | ES                 | SZ                | RF                  | RID             | Count          |
| C6                 | C6                 | 6                 | C6                  | 46.150.18       | 1              |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3        | 1              |
| C6-C6              | C6-C6              |                   |                     |                 |                |



D1—O—Et

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 84:91652 CA  
 TI Polycyclic dyes  
 IN Groll, Manfred; Hederich, Volker; Bien, Hans S.  
 PA Bayer A.-G., Fed. Rep. Ger.  
 SO Ger. Offen., 38 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 IC C08K  
 CC 40-6 (Dyes, Fluorescent Whiteners, Agents, and Photosensitizers)  
 FAN.CNT 1

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|-------------|------|----------|-----------------|----------|
| DE 2424542  | A1   | 19751211 | DE 1974-2424542 | 19740521 |
| GB 1451304  | A    | 19760929 | GB 1975-18965   | 19750506 |
| CH 613986   | A    | 19791031 | CH 1977-655     | 19750516 |
| JP 50161523 | A2   | 19751227 | JP 1975-58772   | 19750519 |
| US 4024144  | A    | 19770517 | US 1975-578770  | 19750519 |
| FR 2272152  | A1   | 19751219 | FR 1975-15846   | 19750521 |
| FR 2272152  | B1   | 19790330 |                 |          |

PRAI DE 1974-2424542 19740521

GI For diagram(s), see printed CA Issue.

AB Isomeric mixts. of polycyclic dyes (I R = H, iso-C8H17; X = o-phenylene,

naphthylene; X1 = X, substituted 1,8-naphthylene or o-phenylene) and their brominated derivs. were prepared and used to dye polyester fibers fast yellow to red shades. Thus, a mixture of o-C6H4(NH2)2 [95-54-5] and 3-(phenoxy sulfonyl)naphthalic anhydride [58370-80-2] in HOAc was refluxed until the reaction was completed, the solution cooled, and II [58370-90-4] and its isomer [58370-91-5] were isolated. The other I were similarly prepared

ST phenyl polycyclic sulfonate dye; polyester fiber dye; isoquinoline sulfonate ester dye; perinone dye; phthaloperinone dye; naphthoylenebenzimidazole dye

IT Polyester fibers  
RL: USES (Uses)  
(dyes for, naphthoylenebenzimidazole and phthaloperinone sulfo derivs.  
as)

IT Dyes  
(naphthoylenebenzimidazole and phthaloperinone sulfo derivs., polyester fibers)

IT 14H-Benz[4,5]isoquino[2,1-a]perimidine-12-sulfonic acid, 14-oxo-, phenyl ester, bromo derivative  
14H-Benz[4,5]isoquino[2,1-a]perimidine-9-sulfonic acid, 14-oxo-, phenyl ester, bromo derivative  
7H-Benzimidazo[2,1-a]benz[de]isoquinoline-2-sulfonic acid, 7-oxo-, phenyl ester, bromo derivative  
7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 7-oxo-, phenyl ester, bromo derivative  
RL: TEM (Technical or engineered material use); USES (Uses)  
(dye, for polyester fibers, preparation of)

IT 58370-86-8 58370-87-9 58370-88-0 58370-89-1 58370-90-4  
58370-91-5 58373-84-5 58373-85-6 58373-89-0 58373-90-3  
58373-91-4 58373-92-5 58374-12-2 58374-13-3 58676-84-9  
RL: TEM (Technical or engineered material use); USES (Uses)  
(dye, for polyester fibers, preparation of)

IT 58373-88-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with phenol)

IT 1197-37-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with (phenoxy sulfonyl)naphthalic acid derivative)

IT 95-54-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with (phenoxy sulfonyl)naphthalic anhydride)

IT 479-27-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with (phenoxy sulfonyl)phthalic acid)

IT 58370-80-2 58370-81-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diaminoaryl derivs.)

IT 58374-11-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diaminonaphthalene)

IT 58370-83-5 58370-84-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diaminophenetole)

IT 58370-85-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with naphthalenediamine)

IT 58373-86-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with naphthylenediamine)

IT 58373-87-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phosphorus oxychloride)

IT 58370-82-4

IT      RL: RCT (Reactant); RACT (Reactant or reagent)  
          (reaction of, with sodium phenoxide)

IT      139-02-6

IT      RL: USES (Uses)  
          (reaction with (chlorosulfonyl)naphthalic anhydride)

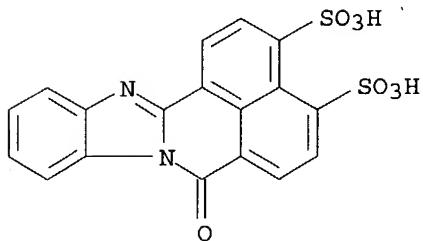
IT      108-95-2, reactions

IT      RL: RCT (Reactant); RACT (Reactant or reagent)  
          (with phthaloperinonesulfonyl chloride)

RN 64193-49-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3,4-disulfonic acid, 7-oxo-,  
     disodium salt (9CI) (CA INDEX NAME)  
 MF C18 H10 N2 O7 S2 . 2 Na  
 LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier | RID Occurrence |
|--------------------|--------------------|-------------------|---------------------|-----------------|----------------|
| EA                 | ES                 | SZ                | RF                  | RID             | Count          |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3        | 1              |
| C6-C6              | C6-C6              |                   |                     |                 |                |



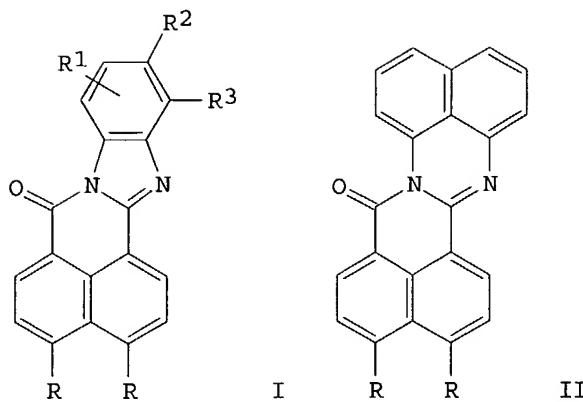
● 2 Na

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 87:153423 CA  
 TI Water-soluble dyes for wool  
 IN Imahori, Seiichi; Murata, Yukichi; Maeda, Shuichi  
 PA Mitsubishi Chemical Industries Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 4 pp.  
     CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC C09B057-00  
 CC 40-6 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)  
 FAN.CNT 1  

| PATENT NO.          | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------------|------|----------|-----------------|----------|
| PI JP 52072726      | A2   | 19770617 | JP 1975-149840  | 19751216 |
| JP 58057463         | B4   | 19831220 |                 |          |
| PRAI JP 1975-149840 |      | 19751216 |                 |          |
| GI                  |      |          |                 |          |



AB The title dyes I ( $R = SO_3Na$ ;  $R1 = H, Me, OMe, NO_2$ ;  $R2, R3 = H$  or  $R2R3 = benzo$ ) and II ( $R = SO_3Na$ ) [64193-50-6] were prepared by reaction of  $Na_2O_3$  with I ( $R = Cl, Br$ ) and II ( $R = Cl$ ) [40445-16-7]. For example, I ( $R = Cl$ ,  $R1 = R2 = R3 = H$ ) [40445-12-3] was autoclaved with aqueous  $Na_2SO_3$  at  $150^\circ$  for 20 h and salted to give I ( $R = SO_3Na$ ,  $R1 = R2 = R3 = H$ ) [64193-49-3], reddish yellow on wool.

ST oxobenzimidazobenzisoquinolinedisulfonate dye wool;  
oxobenzisoquinoperimidinedisulfonate dye wool

IT Dyes  
 (oxobenzimidazobenzisoquinolinedisulfonates and  
 oxobenzisoquinoperimidinedisulfonates, with high solubility, for wool)

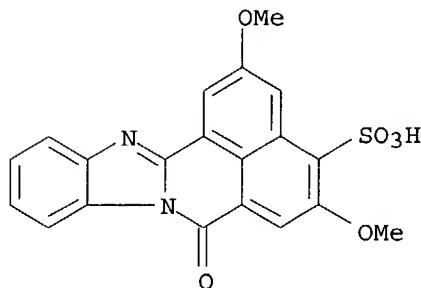
IT 64190-18-7P    64190-19-8P    64190-20-1P    64193-47-1P    64193-49-3P  
 64193-50-6P  
 RL: MSC (Miscellaneous); PREP (Preparation)  
 (dyes, highly soluble, for wool, manufacture of)

IT 40445-12-3    40445-16-7    64190-10-9    64190-21-2    64190-22-3  
 64193-48-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (sulfonation of)

RN 62599-18-2 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-4-sulfonic acid,  
 2,5-dimethoxymethyl-7-oxo-, sodium salt (9CI) (CA INDEX NAME)  
 MF C21 H16 N2 O6 S . Na  
 CI IDS  
 LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier | RID Occurrence |
|--------------------|--------------------|-------------------|---------------------|-----------------|----------------|
| EA                 | ES                 | SZ                | RF                  | RID             | Count          |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3        | 1              |
| C6-C6              | C6-C6              |                   |                     |                 |                |



D1—Me

● Na

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

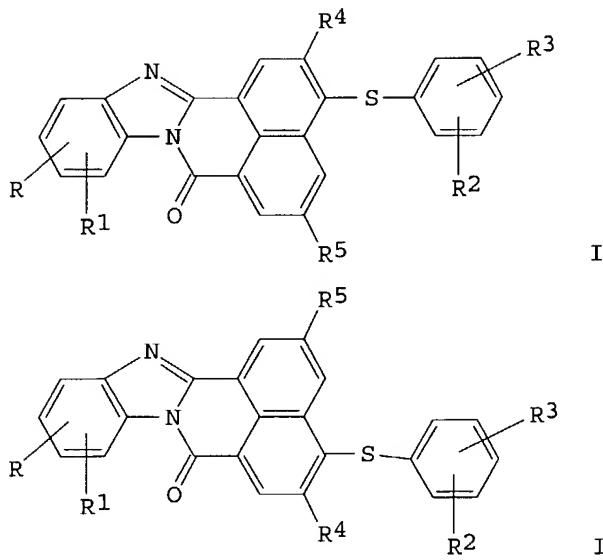
REFERENCE 1

AN 86:191337 CA  
 TI 1,8-Naphthoylenebenzimidazole derivatives  
 IN Shiroasaki, Tsutomu  
 PA Nippon Kayaku Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC C09B057-00  
 CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)  
 Section cross-reference(s): 28

FAN.CNT 1

| PATENT NO.         | KIND  | DATE     | APPLICATION NO. | DATE     |
|--------------------|-------|----------|-----------------|----------|
| -----              | ----- | -----    | -----           | -----    |
| PI JP 51111237     | A2    | 19761001 | JP 1975-36069   | 19750327 |
| PRAI JP 1975-36069 |       | 19750327 |                 |          |

GI



AB I-II mixts. ( $R = H, Me, OMe, Bu, NO_2, Cl, CO_2H; R1 = H, Me; R2 = H, NH_2, Bu, Me, OMe; R3 = H, Cl, Me, CO_2H; R4 = H, Cl, Br, OH, OMe, OPr; R5 = H, Cl, Br, OH, OMe, OPr, NO_2, SO_2NMe_2, SO_2NET_2$ ) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared. For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at  $98^\circ$  for 12 h and then autoclaved with 2-aminobenzenethiol [137-07-5] in the presence of  $K_2CO_3$  and  $Na_2SO_3 \cdot 7H_2O$  at  $150^\circ$  for 10 h and at  $170^\circ$  for 12 h to give I-II mixture (all  $R$ 's =  $H$  except  $R2 = 2-NH_2$ ); about 34 I-II mixts. were prepared.

ST phenylthionaphthoylenebenzimidazole deriv manuf; naphthoylenebenzimidazole phenylthio deriv

IT Dyes  
 (intermediates, (phenylthio)naphthoylenebenzimidazole derivs.)

IT 41537-57-9P 62602-99-7P  
 RL: PREP (Preparation)  
 (manufacture and reaction with aminobenzenethiol)

IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P  
 RL: PREP (Preparation)  
 (manufacture and reaction with aminomethylbenzenethiol)

IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P  
 62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P  
 62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P  
 62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P  
 62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P  
 62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P  
 62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P  
 62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P  
 62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P  
 62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P  
 62599-24-0P 62599-25-1P 62599-26-2P 62599-27-3P 62599-28-4P  
 62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P  
 62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P  
 62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P  
 RL: IMF (Industrial manufacture); PREP (Preparation)  
 (preparation of)

IT 62635-64-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with benzenediamine)

IT 95-54-5, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthalic anhydride sodium salt)

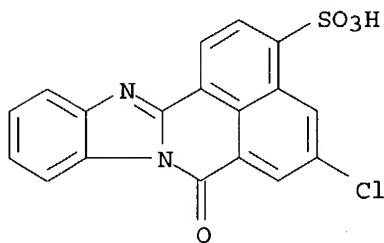
IT 106-45-6 137-07-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole)

IT 2396-68-1 23451-96-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole derivs.)

RN 62599-40-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3-sulfonic acid,  
     5-chloromethyl-7-oxo-, sodium salt (9CI) (CA INDEX NAME)  
 MF C19 H11 Cl N2 O4 S . Na  
 CI IDS  
 LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier | RID Occurrence |
|--------------------|--------------------|-------------------|---------------------|-----------------|----------------|
| EA                 | ES                 | SZ                | RF                  | RID             | Count          |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3        | 1              |
| C6-C6              | C6-C6              |                   |                     |                 |                |



D1-Me

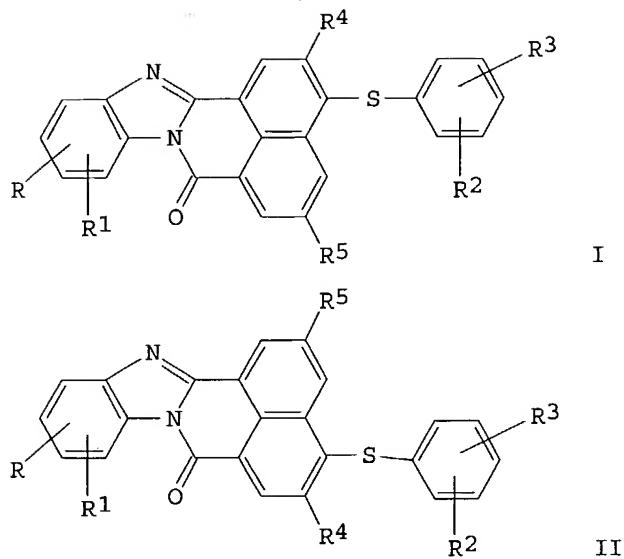
● Na

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:191337 CA  
 TI 1,8-Naphthoquinolenebenzimidazole derivatives  
 IN Shiroasaki, Tsutomu  
 PA Nippon Kayaku Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC C09B057-00  
 CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)  
     Section cross-reference(s): 28  
 FAN.CNT 1  

| PATENT NO.         | KIND  | DATE     | APPLICATION NO. | DATE     |
|--------------------|-------|----------|-----------------|----------|
| -----              | ----- | -----    | -----           | -----    |
| PI JP 51111237     | A2    | 19761001 | JP 1975-36069   | 19750327 |
| PRAI JP 1975-36069 |       | 19750327 |                 |          |
| GI                 |       |          |                 |          |



AB I-II mixts. ( $R = H, Me, OMe, Bu, NO_2, Cl, CO_2H; R1 = H, Me; R2 = H, NH_2, Bu, Me, OMe; R3 = H, Cl, Me, CO_2H; R4 = H, Cl, Br, OH, OMe, OPr; R5 = H, Cl, Br, OH, OMe, OPr, NO_2, SO_2NMe_2, SO_2NET_2$ ) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared. For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at  $98^\circ$  for 12 h and then autoclaved with 2-aminobenzenethiol [137-07-5] in the presence of  $K_2CO_3$  and  $Na_2SO_3 \cdot 7H_2O$  at  $150^\circ$  for 10 h and at  $170^\circ$  for 12 h to give I-II mixture (all  $R$ 's =  $H$  except  $R2 = 2-NH_2$ ); about 34 I-II mixts. were prepared.

ST phenylthionaphthylenebenzimidazole deriv manuf; naphthylenebenzimidazole phenylthio deriv

IT Dyes  
(intermediates, (phenylthio)naphthylenebenzimidazole derivs.)

IT 41537-57-9P 62602-99-7P  
RL: PREP (Preparation)  
(manufacture and reaction with aminobenzenethiol)

IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P  
RL: PREP (Preparation)  
(manufacture and reaction with aminomethylbenzenethiol)

IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P  
62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P  
62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P  
62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P  
62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P  
62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P  
62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P  
62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P  
62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P  
62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P  
62599-24-0P 62599-25-1P 62599-26-2P 62599-27-3P 62599-28-4P  
62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P  
62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P  
62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of)

IT 62635-64-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with benzenediamine)

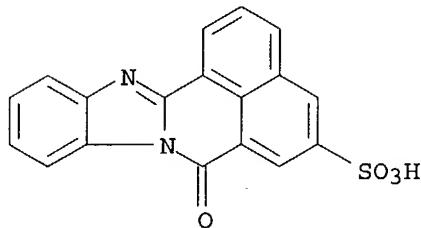
IT 95-54-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sulfonaphthalic anhydride sodium salt)  
IT 106-45-6 137-07-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole)  
IT 2396-68-1 23451-96-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfonaphthoylenebenzimidazole derivs.)

RN 521307-85-7 REGISTRY  
 ED Entered STN: 28 May 2003  
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 7-oxo- (9CI)  
     (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H10 N2 O4 S  
 SR CA  
 LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis | Elemental Sequence | Size of the Rings | Ring System Formula | Ring Identifier RID | RID Occurrence Count |
|--------------------|--------------------|-------------------|---------------------|---------------------|----------------------|
| EA                 | ES                 | SZ                | RF                  | RID                 |                      |
| C3N2-C5N-C6-       | NCNC2-NC5-C6-      | 5-6-6-6-6         | C18N2               | 6841.6.3            | 1                    |
| C6-C6              | C6-C6              |                   |                     |                     |                      |



Calculated Properties (CALC)

| PROPERTY (CODE)              | VALUE            | CONDITION  | NOTE    |
|------------------------------|------------------|------------|---------|
| Bioconc. Factor (BCF)        | 1                | pH 1       | (1) ACD |
| Bioconc. Factor (BCF)        | 1                | pH 4       | (1) ACD |
| Bioconc. Factor (BCF)        | 1                | pH 7       | (1) ACD |
| Bioconc. Factor (BCF)        | 1                | pH 8       | (1) ACD |
| Bioconc. Factor (BCF)        | 1                | pH 10      | (1) ACD |
| Freely Rotatable Bonds (FRB) | 2                |            | (1) ACD |
| H acceptors (HAC)            | 6                |            | (1) ACD |
| H donors (HD)                | 1                |            | (1) ACD |
| Koc (KOC)                    | 5.50             | pH 1       | (1) ACD |
| Koc (KOC)                    | 2.88             | pH 4       | (1) ACD |
| Koc (KOC)                    | 1                | pH 7       | (1) ACD |
| Koc (KOC)                    | 1                | pH 8       | (1) ACD |
| Koc (KOC)                    | 1                | pH 10      | (1) ACD |
| logD (LOGD)                  | 0.93             | pH 1       | (1) ACD |
| logD (LOGD)                  | 0.65             | pH 4       | (1) ACD |
| logD (LOGD)                  | -0.65            | pH 7       | (1) ACD |
| logD (LOGD)                  | -0.67            | pH 8       | (1) ACD |
| logD (LOGD)                  | -0.67            | pH 10      | (1) ACD |
| logP (LOGP)                  | 3.430+/-0.620    |            | (1) ACD |
| Molar Solubility (SLB.MOL)   | <0.01 mol/L      | pH 1       | (1) ACD |
| Molar Solubility (SLB.MOL)   | <0.01 mol/L      | pH 4       | (1) ACD |
| Molar Solubility (SLB.MOL)   | >=0.1 - <1 mol/L | pH 7       | (1) ACD |
| Molar Solubility (SLB.MOL)   | >=0.1 - <1 mol/L | pH 8       | (1) ACD |
| Molar Solubility (SLB.MOL)   | >=0.1 - <1 mol/L | pH 10      | (1) ACD |
| Molecular Weight (MW)        | 350.35           |            | (1) ACD |
| pKa (PKA)                    | 4.00+/-0.20      | Most Basic | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:370267 CA  
TI Soluble polycyclic dyes  
AU Wolska, Anna; Wojciechowski, Krzysztof; Niewiadomski, Zbigniew  
CS Inst. Barwnikow i Produktow Org., Zgierz, 95-100, Pol.  
SO Barwniki, Srodki Pomocnicze (2002), 46(1/2), 15-26  
CODEN: BSPOEM; ISSN: 0867-7824  
PB Instytut Barwnikow i Produktow Organicznych  
DT Journal  
LA Polish  
CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic  
Sensitizers)  
Section cross-reference(s): 40, 28  
AB The article describes the preparation of soluble polycyclic dyes containing  
imide or  
imidazole moieties and the possibility to using them for dyeing cellulosic  
fibers as direct dyes. The dyes were obtained by condensation of  
1,8-naphthalenedicarboxylic acid, 1,4,5,8-naphthalenetetracarboxylic acid,  
or 3,4,9,10-perylenetetracarboxylic acid with aniline or  
o-phenylenediamine, followed by sulfonation of the condensation products.  
Depending on the dye type, cotton fabric was dyed to attain yellow, blue,  
or orange color. The importance of sulfonation conditions in obtaining  
dyes with good vat dyeing properties is discussed.  
ST polycyclic vat dye prepn cotton fabric dyeing; sulfonated imide imidazole  
group contg polycyclic vat dye prepn  
IT Textiles  
(cotton; preparation of polycyclic vat dyes and their use in cotton fabric  
dyeing)  
IT Sulfonation  
(effect of sulfonation conditions on preparation of polycyclic vat dyes and  
use of the obtained dyes in cotton fabric dyeing)  
IT Vat dyeing  
(preparation of polycyclic vat dyes and their use in cotton fabric dyeing)  
IT Dyes  
(vat; preparation of polycyclic vat dyes and their use in cotton fabric  
dyeing)  
IT 440093-45-8P 440093-46-9P 521307-84-6P 521307-85-7P 521307-86-8P  
521963-64-4P 521963-65-5P  
RL: CPS (Chemical process); PEP (Physical, engineering or chemical  
process); PRP (Properties); SPN (Synthetic preparation); TEM (Technical or  
engineered material use); PREP (Preparation); PROC (Process); USES (Uses)  
(dye; preparation of polycyclic vat dyes and their use in cotton fabric  
dyeing)  
IT 128-65-4P 4216-02-8P 4424-06-0P 23749-58-8P 55034-79-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate in dye preparation; preparation of polycyclic vat dyes and  
their  
use in cotton fabric dyeing)  
IT 62-53-3, Aniline, reactions 81-30-1 85-44-9, Phthalic anhydride  
95-54-5, o-Phenylenediamine, reactions 128-69-8 6914-98-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant in dye preparation; preparation of polycyclic vat dyes and their  
use in

cotton fabric dyeing)